EFFECT OF ELECTRONIC STRUCTURE ON PHASE EQUILIBRIA IN THE AlB2-ScB2-YB2-ZrB2-HfB2-NbB2-TaB2 SYSTEM

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Compositions in the AlB_2-ScB_2-YB_2-ZrB_2-HfB_2-NbB_2-TaB_2 system were selected to determine the effect of electronic structure on phase equilibria and solid solubility. The Group IVB diborides have the highest stability considering a melting point criterion (eg., ZrB_2 with 10 valence electrons per unit cell, or 10 e-/uc) and three systems were investigated to characterize phase equilibria at or near this optimum valence electron sum. The materials were synthesized by hot-pressing diboride powder mixtures at 1750°C followed by heat-treatments at 1900 and 2000°C. The compositions in the system $xScB_2$-$(1-x)TaB_2$ (varying from 9 to 11 e-/uc, respectively), with a metal atom radius difference of 7.4%, exhibited complete solid solubility that could be attributed to the change of the net valence electron sum toward the optimum 10 e-/uc value. The $xScB_2$-$(1-x)ZrB_2$ system (varying from 9 to 10 e-/uc, respectively) was found to be quasi-binary, but exhibited insignificant solid solubility despite the metal atom radius of Sc being smaller than Zr by only 1.2%. The lack of solubility is attributed to an electronic structure based incompatibility. The system $x(ZrB_2)$-$(1-x)(0.5ScB_2 - 0.5TaB_2)$, with a valence electron sum of 10 e-/uc for all x, exhibited complete solid solubility. Very similar results were found for the YB2-ZrB2-TaB_2 system, with the exception that significant solubility of ZrB_2 in YB_2 was observed. The unidirectional solubility is attributed to an electronic structure based stabilization of the YB_2. The compatibilities observed for all compositions investigated indicate that ZrB_2-ScB_2-TaB_2 and ZrB_2-YB_2-TaB_2 are quasi-ternary systems. Additional 4, 5, and 6 component diboride systems with an average valence sum of 10 e-/fu were also investigated in the AlB_2-ScB_2-YB_2-ZrB_2-HfB_2-NbB_2-TaB_2 system, and many formed solid solutions. The results confirm the significance of electronic structure for phase equilibria and solid solubilities for these diborides. The solid solutions also provide a basis for further investigations as high entropy boride systems